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LIFE Chamber Chemical Equilibrium Simulations with Additive Hydrogen, Oxygen, and Nitrogen

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Disclaimer

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1. Abstract

In order to enable continuous operation of a Laser Inertial confinement Fusion Energy (LIFE) engine, the material (fill-gas and debris) in the fusion chamber must be carefully managed. The chamber chemical equilibrium compositions for post-shot mixtures are evaluated to determine what compounds will be formed at temperatures 300-5000K. It is desired to know if carbon and or lead will deposit on the walls of the chamber, and if so: at what temperature, and what elements can be added to prevent this from happening. The simulation was conducted using the chemical equilibrium solver Cantera with a Matlab front-end . Solutions were obtained by running equilibrations at constant temperature and constant specific volume over the specified range of temperatures. It was found that if nothing is done, carbon will deposit on the walls once it cools to below 2138K, and lead below 838K. Three solutions to capture the carbon were found: adding pure oxygen, hydrogen/nitrogen combo, and adding pure nitrogen. The best of these was the addition of oxygen which would readily form CO at around 4000K. To determine the temperature at which carbon would deposit on the walls, temperature solutions to evaporation rate equations needed to be found. To determine how much carbon or any species was in the chamber at a given time, chamber flushing equations needed to be developed. Major concerns are deposition of carbon and/or oxygen on the tungsten walls forming tungsten oxides or tungsten carbide which could cause embrittlement and cause failure of the first wall. Further research is needed.

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2. Introduction

The LIFE Chamber Chemical Equilibrium Study was performed to better understand the different compounds that would form when a target of specified composition was ignited inside the chamber at various temperatures ranging from 300 to 5000K. A chemical equilibrium solver, Cantera, was used to solve for the compound distributions inside the chamber. In equilibration Cantera minimizes the free energy of the system by distributing individual atoms among a pre-defined list of compounds at a specified temperature and specific volume. Specific heat data fits are taken from the NASA Thermo Tables and are used by Cantera to calculate Gibbs free energy for all the possible compounds.

In the LIFE chamber, there will be an initial density of Xenon at $4\frac{g}{m^3}$, into which a hohlraum will be injected and ignited. The temperatures will reach levels of 5000K or higher initially, but will immediately cool. As the components of the hohlraum cool they will begin to form compounds or condense/solidify onto the surrounding cooler walls of the system. The main concern is that for a hohlraum made of Pb, C, Ta, N, O, H, D, and T, the Lead and the Carbon would condense or deposit respectively on the walls of the chamber. Tantalum could

also be an issue, however, for this study, Tantalum is assumed to be in such low quantities that it can be assumed negligible.

There will be some particles that do hit the walls, and assuming no wall reactions take place, there will be a lower bound limiting temperature for deposition on the walls based upon input mass rate, chamber surface area, and species evaporation rates. The purpose of this study was to determine what the limits are for Carbon and Lead evaporation rates, and to determine if it is possible to form compounds with Lead or Carbon before the evaporation limit is reached, that would stay gaseous and not collect on the walls of the chamber at cooler temperatures.

3. Setup Analysis/Modeling

3.1 Limitations and Evaporations Rates

In order to better gauge the scope of this simulation it is necessary to know the constraints of the code used. The Cantera equilibrium solver minimizes the free energy in the gas phase only; therefore, any reaction that would normally take place when a component is in a liquid or solid phase cannot be modeled by this simulation. The results from simulations where this occurs must then be considered non-physical. In addition to only being valid in the gas phase, Cantera will consider all the components that it is given to always be in the gas phase so it is thus important to know the limiting temperatures for all species that would collect on the walls, and under what conditions. For the temperature range of 300-5000K, at densities around $4\frac{g}{m^3}$, the only species that will collect on the walls are Carbon, Lead, and Tantalum. Because of the minute amounts of Tantalum in the target composition used in this simulation it can be neglected, however evaporation limit calculations were still performed for all three species. The evaporation limit, as defined in this context, is the temperature at which the rate of input mass of an atomic species is equal to the evaporation rate of atoms from the surface. The evaporation rate is given by (1):

$$W\left(\frac{g}{m^2 \cdot s}\right) = 10^{A-\frac{B}{T}-0.5\log T+C} \qquad (3.1)$$

Where constants A, B, and C are given by Table 3.1 (1):

	A	B	C
Carbon	14.06	38570	0.3056
Lead	10.69	9600	0.9242
Tantalum	13.00	40210	0.8947

Table 3.1: Constants in the Equation for the Rate of Evaporation for Carbon, Lead, and Tantalum.

Hence, for a given input mass rate for each component, an evaporation rate can be found if the surface area inside the chamber is known. An equilibrium evaporation temperature can then be solved for iteratively (See Appendix A.2.1 for MatLab code). Assumptions made in this calculation are 2.5m radius spherical chamber, ideal gas behavior, and a shot rate of 10

hohlraums per second. Lastly, the Cantera equilibrium solver will only consider the compounds that it is given. A list of possible compounds was formulated by taking only those compounds that are readily formed.

Element	H	He	C	N	O	Xe	Ta	Pb
Compounds	H_2, HCN, H_2O		CH_2, CH_3, CH_4, CN, CO, CO_2, C_3H_8	NH_3, NO, N_2	OH, O_2		TaO, TaO_2	PbH, PbO, Pb_2

Table 3.2: Elements and Their Compounds

3.2 Test Cases

Five test scenarios were run, one base case, and 4 test cases with different additive elements included in the bulk chamber gas. In the base case scenario, the chamber is assumed to be fully populated with Xe gas at $4\frac{g}{m^3}$. A Hohlraum is then injected into the chamber and ignited. Using a 30% fusion burn factor, 30% of the DT fuel is converted to Helium and all the elements are entered into Cantera. In order to determine trends based on temperature, equilibration is done at constant temperature and specific volume for different temperatures from 300 to 5000K in steps of 50K for a given initial composition. In Cases 1-4, Hydrogen, Oxygen, Nitrogen, and Nitrogen-Hydrogen combinations are added to the Xenon bulk gas respectively.

Element	Pb	DT	H	Ta	C	N	O
Mass (mg)	398	0.34	7.6e-4	2.1e-3	5.6	9.7e-4	3.7e-3

Table 3.3: Total Elemental Masses in Sample LIFE Target.

3.3 Chamber Gas Flushing Rates

Analysis on the effect of gas flushing rates was also conducted. There are two bounding schemes for determining the amount of hohlraum left in the chamber given a specified flushing fraction of the chamber gas. Both of these methods were initially proposed by R. Moir (2), the following will serve to flush out the details.

3.3.1 Flushing Method 1: Mixed

In the first flushing method, after each shot (Δm) mass is added to the system holding the specific volume constant. The gas is then well mixed. The act of expelling gas makes no change to the equation since if solving for density, and if the gas is well mixed, there will be no change to the density after removing a fixed volume of mass. The initial density and initial mass with volume V is given by:

$$\rho_o = \frac{m_o}{V} \qquad eq.3.2$$

Injecting and igniting one hohlraum gives:

$$\rho_o' = \frac{m_o + \Delta m}{V} \qquad eq.3.3$$

Flushing with some fraction of Xe gas, where x is the fraction of gas remaining and 1-x is the fraction of gas cleared:

$$\rho_1 = \frac{m_o + \Delta m + m_o(1-x)}{V + V(1-x)} = \frac{m_o(2-x) + \Delta m}{V(2-x)} \qquad eq.3.4$$

Proceeding to the next step, adding one hohlraum and flushing with the same fraction of clearing gas:

$$\rho_2 = \frac{m_o(2-x) + \Delta m + \Delta m + m_o(1-x)}{V(2-x) + V(1-x)} = \frac{m_o(3-2x) + 2\Delta m}{V(3-2x)} \qquad eq.3.5$$

Taken to just after the nth shot:

$$\rho_n V = \frac{m_o(n+1-nx) + n\Delta m}{(n+1-nx)} = m_o + \frac{n}{n(1-x)+1}\Delta m \qquad eq.3.6$$

So as $\lim_{n\to\infty}\left(\frac{n}{n(1-x)+1}\right) = \frac{1}{1-x}$ and hence:

$$\rho_\infty V = m_o + \left(\frac{1}{1-x}\right)\Delta m \qquad eq.3.7$$

3.3.2 Flushing Method 2: Unmixed

In the second chamber flushing method a hohlraum shot is added, mixed, and then a fraction of the gas removed. A fraction of Xe gas equal to that in mass of the gas removed is then added back in.

$$\rho_o = \frac{m_o}{V} \qquad eq.3.2$$

$$\rho_o' = \frac{m_o + \Delta m}{V} \qquad eq.3.3$$

Gas is then exhausted (without mixing with the incoming Xe gas) so removing $\frac{(m_o+\Delta m)(1-x)}{V}$ where x is the fraction remaining gives:

$$\rho_o'' = \frac{(m_o + \Delta m)x}{V} \qquad eq.3.8$$

New Xe gas is added:

$$\rho_o''' = \frac{(m_o + \Delta m)x + m_o(1-x)}{V} = \rho_1 = \frac{x\Delta m + m_o}{V} = \frac{m_1}{V} \qquad eq.3.9$$

$$\rho_2 = \frac{(m_1 + \Delta m)x + m_o(1-x)}{V} = \frac{x^2\Delta m + x\Delta m + m_o}{V} = \frac{m_2}{V} \qquad eq.3.10$$

Carrying the process out to the nth shot:

$$\rho_n V = m_o + \Delta m \sum_{i=1}^{n} x^i \qquad eq.3.11$$

Seeing that the Taylor series expansion of:

$$\sum_{i=0}^{\infty} x^i = \frac{1}{1-x} \qquad eq.3.12$$

It can be shown that:

$$\sum_{i=1}^{\infty} x^i = \frac{1}{1-x} - 1 = \frac{x}{1-x} \qquad eq.3.13$$

Such that:

$$\rho_\infty V = m_o + \left(\frac{x}{1-x}\right)\Delta m \qquad eq.3.14$$

The differences between Chamber Flushing method 1 and method 2 are quite simple, and can readily be seen by taking the difference between the two.

$$\left(m_o + \left(\frac{1}{1-x}\right)\Delta m\right)_{method1} - \left(m_o + \left(\frac{x}{1-x}\right)\Delta m\right)_{method2} = \frac{1-x}{1-x}\Delta m = \Delta m \qquad eq.3.15$$

Hence the Δm multiplier in method 1 will always be larger than in method 2 (at the nth shot, where $n = \infty$) by 1 hohlraum(Δm).

4. Results and Discussion

4.1 Evaporation Limits

In order to find the evaporation limit temperature the surface area of the chamber must be found. At a radius of 2.5m the chamber would have a surface area of 78.54m^2. With given mass input values per element (Table 3.3) per shot, and at 10 shots per second, the total mass flux into the chamber is known. The temperature of the evaporation limit for each atomic species can then be calculated by iteratively evaluating the equations of atomic evaporation rates for temperature, based upon mass flux of Carbon, Tantalum, and Lead. These limits were found to be 2438K for Carbon, 2138K for Tantalum, and 839K for Lead.

4.2 Test Cases Evaluation

For each case run, six plots of data were generated to cover six ranges of various orders of molar magnitudes for each of the compounds. Range 1 was anything greater than 1e-2 moles, ranges 2 to 5 each spanned two orders of magnitude from a max in range 2 of 1e-2 to the min in range 5 of 1e-10. Finally range 6 was anything below 1e-10 moles.

	Range 1	Range 2	Range 3	Range 4	Range 5	Range 6
Span	>1e-2	1e-2 > x > 1e-4	1e-4 > x > 1e-6	1e-6 > x > 1e-8	1e-8 > x > 1e-10	<1e-10

Table 4.1: Data Ranges for Test Case Simulations

Each series was automatically placed in a data range depending on the maximum molar value of the species over the temperature range of 300-5000K. Ranges 1 and 6 are not displayed in the appendices as they consisted primarily of Xe or a filler gas if the levels were high enough or minor species at very low concentrations. Nearly all points of interest are in Range 2 located in the upper left hand corner of the graph. Range 3 is located in the upper right, Range 4 in the bottom left, and Range 5 in the bottom right.

4.2.1 Base Case

In the base case scenario the goal was to see the effects of doing nothing to chamber composition (See appendix A.1.1) and to watch the effects of changing the temperature on the equilibrium composition. In this case the carbon composition is represented by the solid blue line in Range 1. The dip in the carbon levels around 1700K is caused by the formations of hydrocarbons visible in Range. The vertical blue line in Range 1 represents the evaporation limit temperature of Carbon. At temperatures lower than this limit, Carbon will be depositing on the walls faster than it is evaporating. Once carbon becomes deposited on the walls and leaves the gas phase the Cantera solution of it is no longer valid. This is very important as this means that the carbon will have deposited on the walls by 2438K and will no longer be in the gas phase to form compounds below this temperature. Because of this, all the carbon is essentially taken out of the system at 2438K and the hydrocarbons in Range 2 will not form.

Other key points to notice are those dealing with nitrogen and oxygen. In as Range 3, at 4000K, oxygen bonds with carbon to form CO gas. Since this is above carbon's evaporation limit temperature this is a valid simulation and that carbon will get tied up in CO gas. Also note that Nitrogen begins tying up carbon at 3000K in CN gas, and then passes the carbon to HCN at 2000K to end up with HCN gas at lower temperatures. This is also a physical solution as the CN gas is also formed above the evaporation limit of carbon.

4.2.2 Case 1 Adding Hydrogen

In case 1 the addition of Hydrogen gas to the Xe input gas in various ratios relative to the carbon content in the capsule were tested. Full carbon tie-up was achieved at slightly less than a 4:1 Hydrogen to Carbon atomic ratio (See Appendix A.1.2). Simulations were run spanning the range of atomic Hydrogen to Carbon ratios from 1-10. In Case 1 the major hydrocarbons have moved up to Range 1 as compared to Range 2 in the base case, however,

while there is full carbon tie up in CH_4 eventually, it doesn't happen until after the carbon evaporation limit and so it yields a non-physical solution.

4.2.3 Case 2 Adding Oxygen

Case 2 explores the addition of Oxygen gas to the Xenon bulk. Oxygen to Carbon atomic ratios were varied from 0 to 10 over the 300K to 5000K span of temperatures. Full Carbon tie up was achieved in CO at 1x, full Tantalum tie up in TaO was achieved at 1x, and full Lead tie up in PbO was achieved at slightly less than 7x. Appendix A.1.3 shows the results for an oxygen to carbon atomic ratio of 1:1. The carbon is quickly turned to CO around 4000K. All the hydrogen forms H_2 at 1500K which then gets turned to CH_4 scavenging some carbon off of the CO. Key points to note are that between 1500K and 500K all the carbon is tied up as CO, and all the hydrogen is tied up as H_2 with a small amount as H_2O.

In Appendix A.1.4 an oxygen to carbon ration of 7:1 was explored. This case demonstrates full tie-up of Pb in PbO before the evaporation limit of Pb is reached. While this is interesting it may not be useful as PbO has a vapor pressure which is only slightly higher than that of Pb at this temperature. With the excess oxygen it can be seen that around 1500-2500K all the CO is converted to CO_2 as well as all the hydrogen going to H_2O at 1500K.

4.2.4 Case 3 Adding Nitrogen

After examination of Appendix A.1.1, Range 3, it is apparent that nitrogen could also work as a carbon 'getter' as it will form CN around 3000K, however, for nitrogen to tie up a significant amount of carbon before the evaporation limit is reached, copious amounts of nitrogen need to be added. In appendix A.1.5 a nitrogen to carbon atomic ratio of 1:1 is explored. As can be seen in Range 1, the Nitrogen quickly bonds with itself, forming N_2 before finally attaching on the carbon forming CN. At a 1:1 ratio, most of the carbon will deposit on the walls and not make it to the CN gas state as enough of it does not bind up with the nitrogen before the evaporation limit.

To further examine the effects of increasing the nitrogen to carbon ratio on the percentage of overall carbon remaining, all other elements were removed from the simulation and the nitrogen to carbon atomic ratio was varied from 1 to 10,000 (See appendix A.1.6). Hence if 10x nitrogen is added, 30.7% of the carbon will deposit on the walls, at 100x, 11.9% will deposit, at 1,000x, 4.1% will deposit, and at 10,000x, 1.3% will deposit.

Appendix A.1.7 shows a nitrogen to carbon ratio of 1,000:1 where all but 4.1% of the carbon is formed into CN gas. The dip in CN levels at 2000K is caused by the formation of HCN which readily eats at CN until all the hydrogen in the capsule is tied up.

4.2.5 Case 4 Adding Nitrogen and Hydrogen

Because of the vigorously binding nature of Hydrogen with CN gas to form HCN, stoichiometric amounts of Hydrogen and Nitrogen were added to the Xenon fill to attempt to bind up carbon in HCN. First, 1:1 ratios of Nitrogen to Carbon, and Hydrogen to Carbon were added (See Appendix A.1.8). While this had a better Carbon-tie up fraction than just pure Nitrogen, it was still not good enough to successfully tie up all the Carbon. With increasing amounts of Nitrogen and Hydrogen, it is possible to push the HCN curve in Range 1 further to

the right, more readily tying up the Carbon atoms at higher temperatures with increasing production of HCN.

Appendix A.1.9 shows Hydrogen and Nitrogen Carbon ratios of 100x. This drastically lowers the amount of Carbon present, diminishing the carbon to 1.9% of its original value. So with an addition of 200x (combined Nitrogen + Hydrogen atoms at 100x each) the same effect has been achieved as the addition of almost 10,000x of pure Nitrogen. Furthermore, increasing the Nitrogen and Hydrogen levels to 500x each (1,000x total, an increase of a factor of 5) decreases the amount of Carbon left by a factor of 5.68 bringing it down to 0.25% Carbon remaining as can be seen in A.1.10.

4.3 Chamber Gas Flushing Rates

The effect of different chamber gas flushing rates on the composition at the nth shot, where $n = \infty$ is simply a multiplicative factor which, will vary from $1\ to\ \infty$, or $0\ to\ \infty$ depending on the method used. Appendix A.1.11 displays the multiplicative factor for the hohlraum mass Δm for a value of Fraction of Chamber Gas Remaining (x) from 0:0.9 which trends to ∞ as x goes to 1.

5. Conclusion

5.1 Evaporation Limits

The evaporation limits give the lowest possible temperature at which there will be a gas phase of the specified atomic species. While there will be condensation and deposition of the species at higher temperatures, it will evaporate off faster than it is being injected into the chamber.

5.2 Test Case Evaluations

Carbon deposition on the walls is currently considered to be something to avoid. This is important since the first wall, made of Tungsten, reacts readily with carbon to form Tungsten Carbide. Hydrogen does not readily bond with carbon at the high temperatures above carbon's evaporation limit and therefore addition of hydrogen as a carbon 'getter' is not a feasible solution.

The addition of Oxygen to the chamber mixture at a minimum of 1:1 oxygen to carbon atomic ratios will readily tie up all of the carbon at very high temperatures to form CO, and as it cools, CO will bond with oxygen to form CO_2 at around 2000K. The more oxygen that is added, the faster the carbon will be tied up. For better or for worse, the more oxygen that is added in excess of stoichiometric CO will cause the hydrogen to be tied up as H_2O instead of H_2 until all the hydrogen is tied up. It will then proceed to bond with anything it can, after which it will form O_2. The addition of oxygen seems to be the most promising method of binding up the carbon as it does it most readily and at the highest temperatures of all the elements tested in this study.

Adding Nitrogen can be successful in locking up the carbon in CN, however excessively high levels of nitrogen are needed, comparable to those of Xe. To get 4% carbon tie up, nitrogen would have to be at levels close to that of a quarter the number density of xenon (.23 Nitrogen : Xenon ratio). This method is possible, but is estimated to cause problems with such large changes in chamber number density.

By combining Nitrogen and Hydrogen, a hybrid carbon getter can be produced which will first tie up the carbon in CN, but quickly pass it to HCN as it crosses the evaporation limit. As the gas cools, CH_4 becomes the most favorable at around 1000K and carbon gets passes to methane. This method uses only moderate amounts of nitrogen and hydrogen, about 100-500x for each component. At 500-800K all the hydrogen is in H_2 or CH_4 and all the carbon is in CH_4. At 100x nitrogen and hydrogen to carbon ratios the same amount of carbon is tied up as if using pure nitrogen at 10,000x. This would be a second choice method for tying up the carbon as 100x of nitrogen and hydrogen would total to 0.046x the amount of Xenon in the chamber for this configuration.

When exploring the effect of additive elements on Pb composition, only oxygen had any effect at 7x oxygen to carbon atomic ratio. This would lead to the formation of PbO that, while it would stay gaseous at lower temperatures than Pb, initial investigations has found this temperature difference to be small at best (3). Lead will also form compounds with halides such as bromine, chlorine, or iodine. Compounds with these elements could stay gaseous at a significantly lower temperature than Lead; although further research will be needed to better determine that limit. Halide compounds were not initially investigated due to the added complication in equilibrium solutions dealing with all the consequential reactions of the halides with carbon, hydrogen, nitrogen, and oxygen and the compounds that would form subsequently. Mercury which is expected to stay gaseous down to 323K (significantly lower than the limit for Pb), was not investigated, but it is expected to have chemistry similar to that of Pb.

In further research, refinements will need to be made to keep up with the latest target design. If a lot more carbon is added to the target capsule using pure nitrogen would most likely be impossible, and they hydrogen-nitrogen combo would become difficult to use successfully. Further study is needed to determine and to better define the reactions that carbon and oxygen will have with the tungsten walls, and what effects does this have on their lifespan in the chamber.

Various questions still need to be answered. How do small amounts of the product chemical compounds (O_2, H_2, N_2, H_2O, CN, HCN, CH_4, CO, and CO_2) affect laser propagation? How is the hohlraum/Pb material recovered? What else will condense out with Lead in the recovery process? Is it necessary to do hydrogen recovery before or after condensing out the lead?

5.3 Chamber Gas Flushing Rates

The study of the effect of different chamber gas flushing rates on the composition in the chamber as the number of shots approaches infinity is important in determining the bounds on the effects of flushing rates on chamber composition. The actual multiplicative factor used will probably be a combination of the two methods, with method 1 being the most conservative, giving the highest fraction of hohlraum components left in the chamber. The results of this study were not, however, used in the chemical composition calculations since the multiplicative factor for Δm can just be multiplied by the compositions for a given case to get the composition at the nth shot.

6. References

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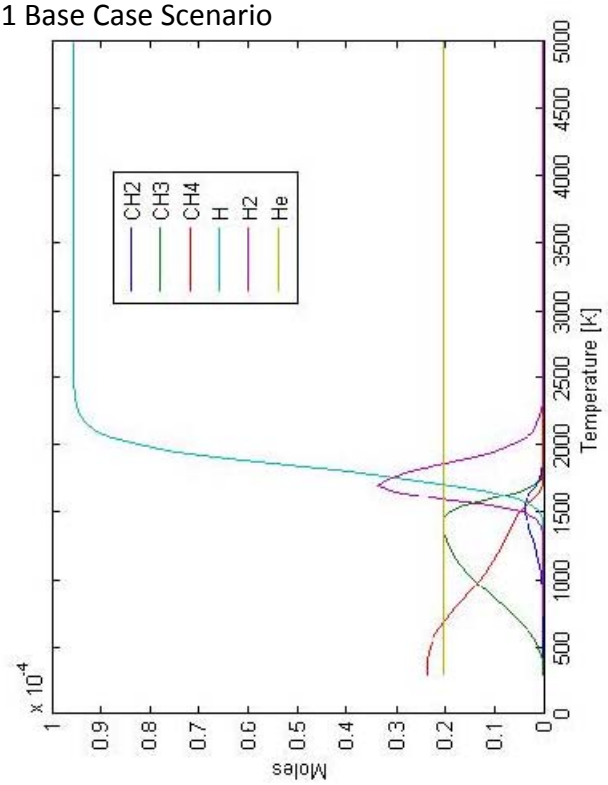
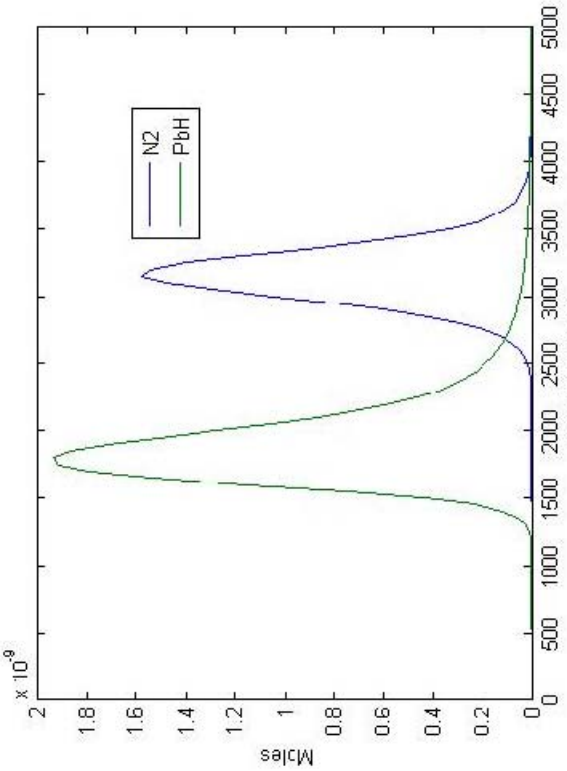
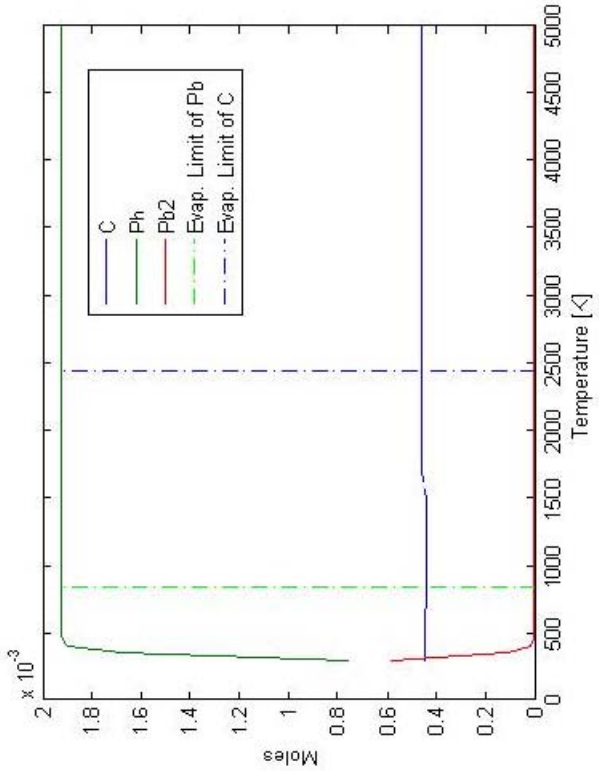
A. Appendix

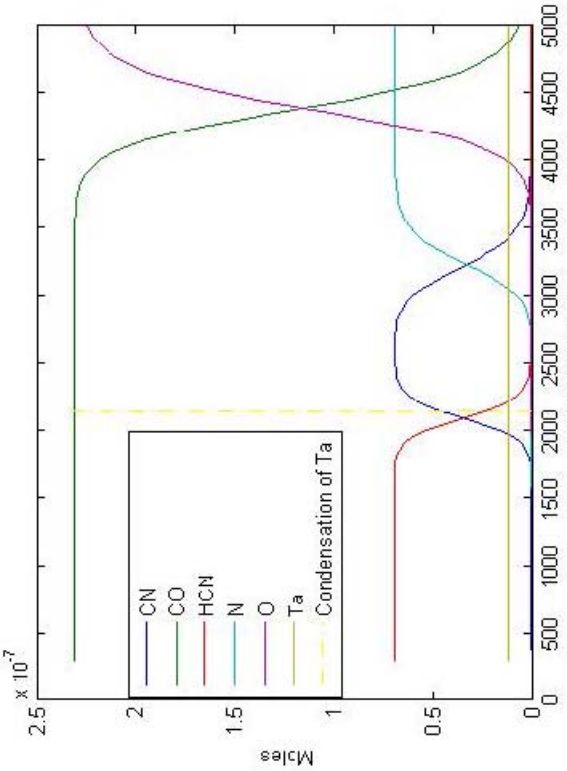
A.1 Graphs

A.1.1 Base Case Scenario

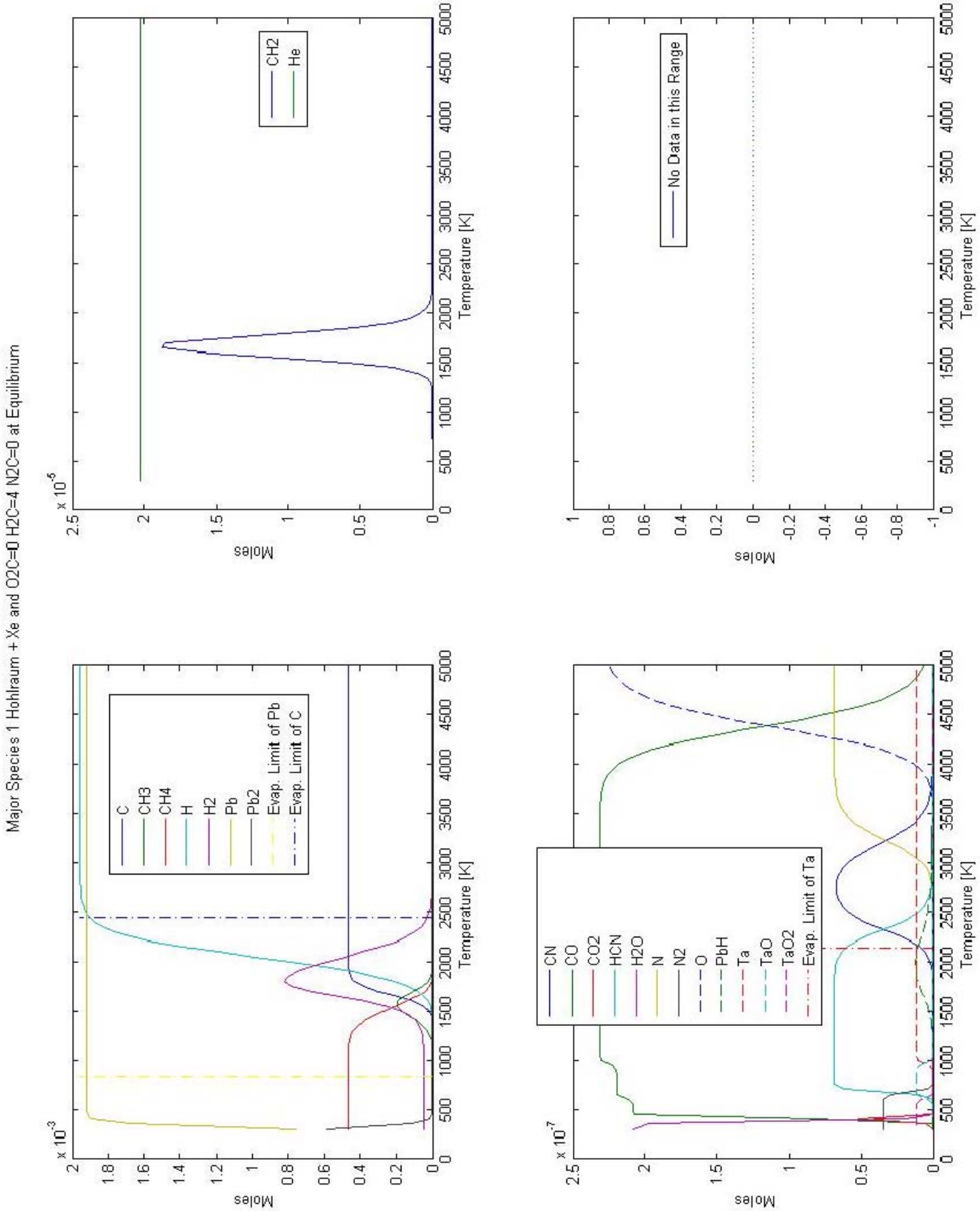




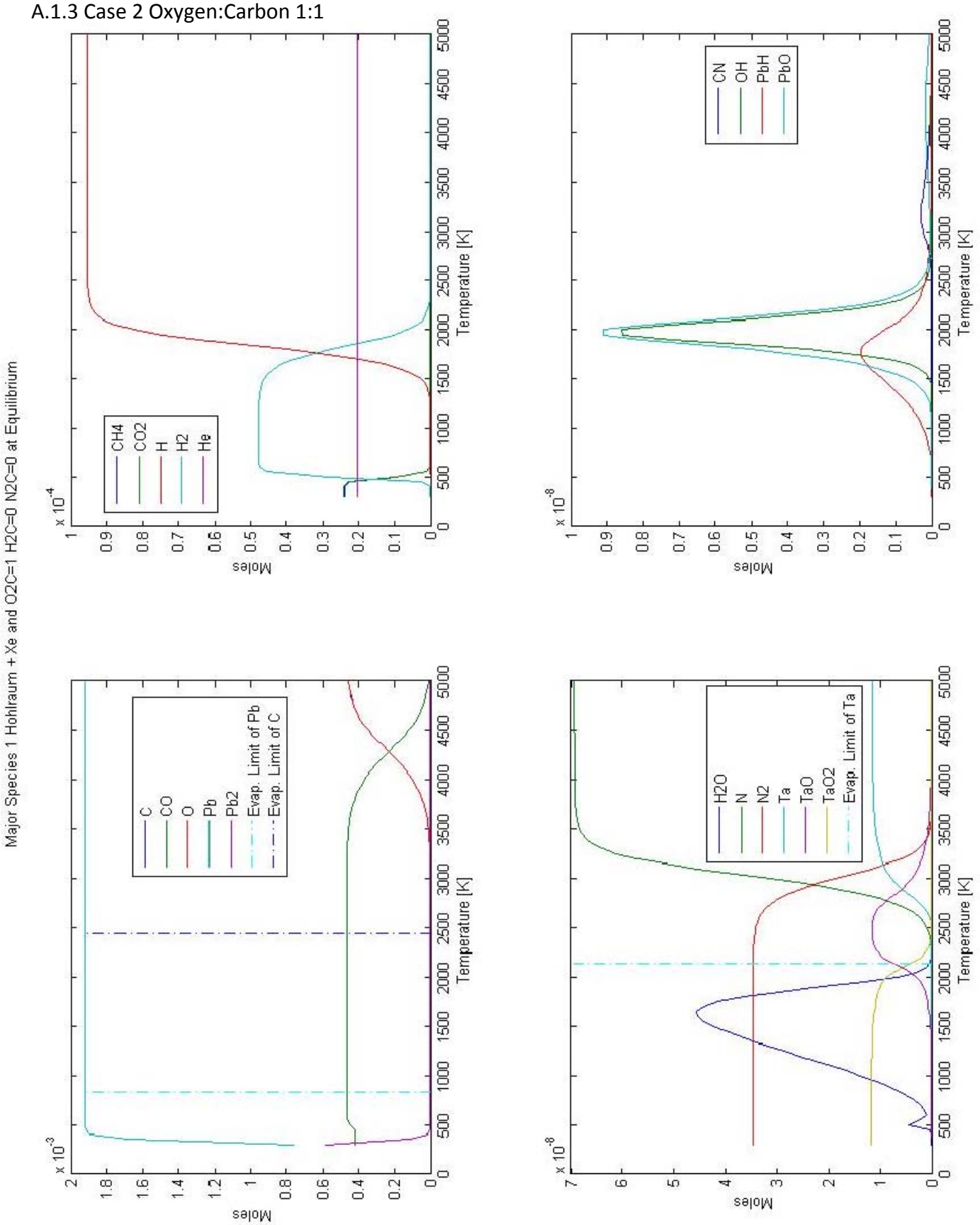




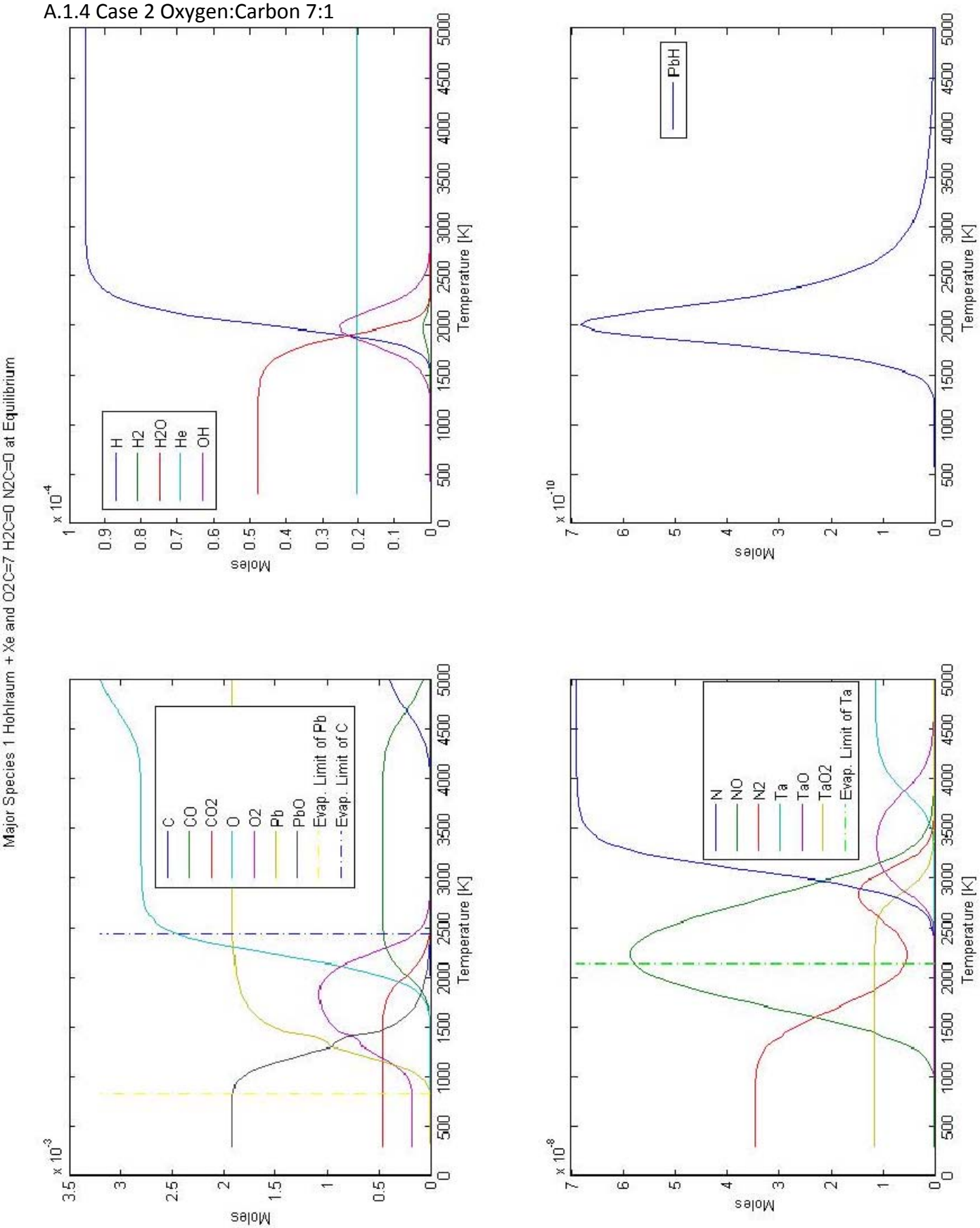
A.1.2 Case 1 Hydrogen:Carbon 4:1



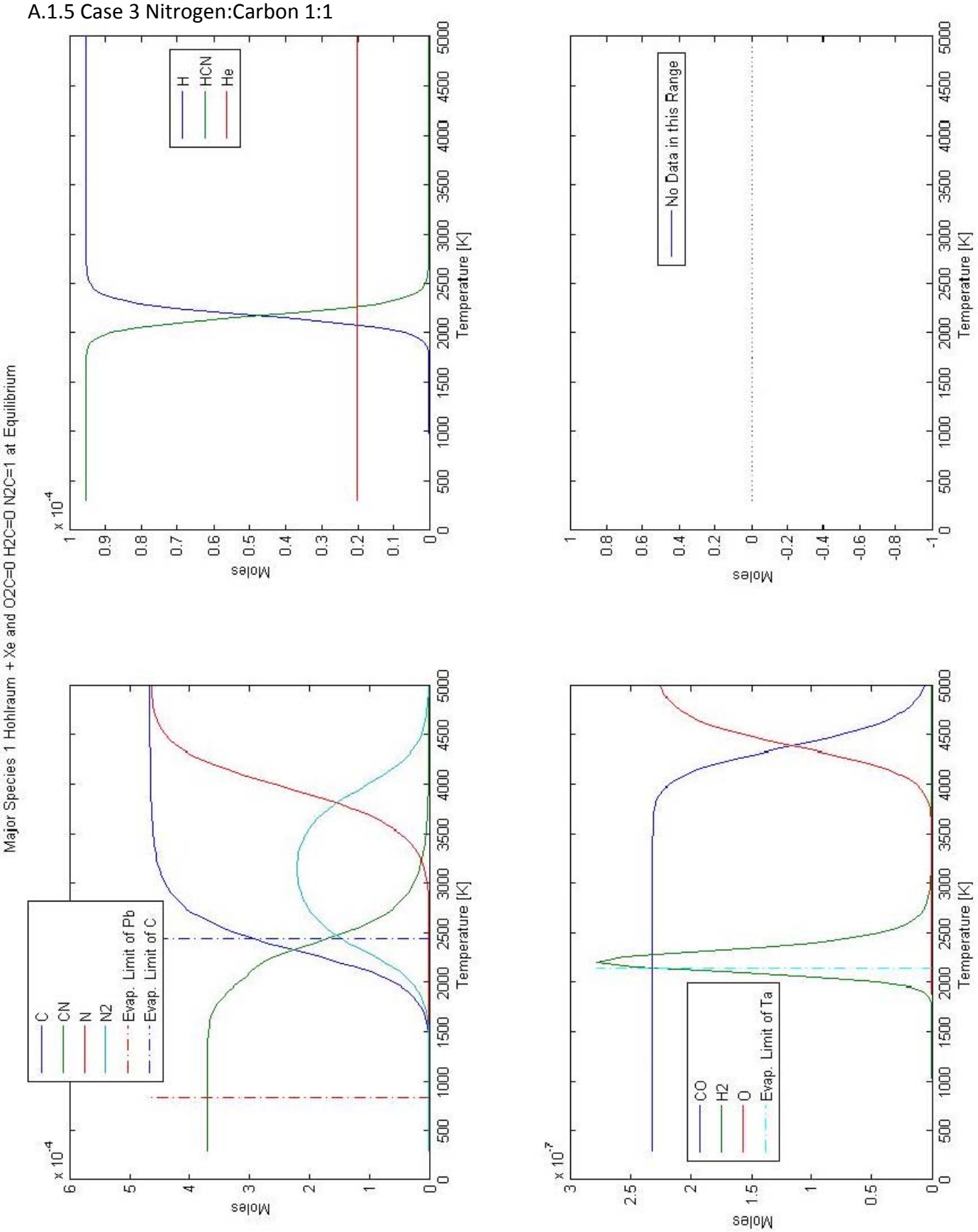
A.1.3 Case 2 Oxygen:Carbon 1:1



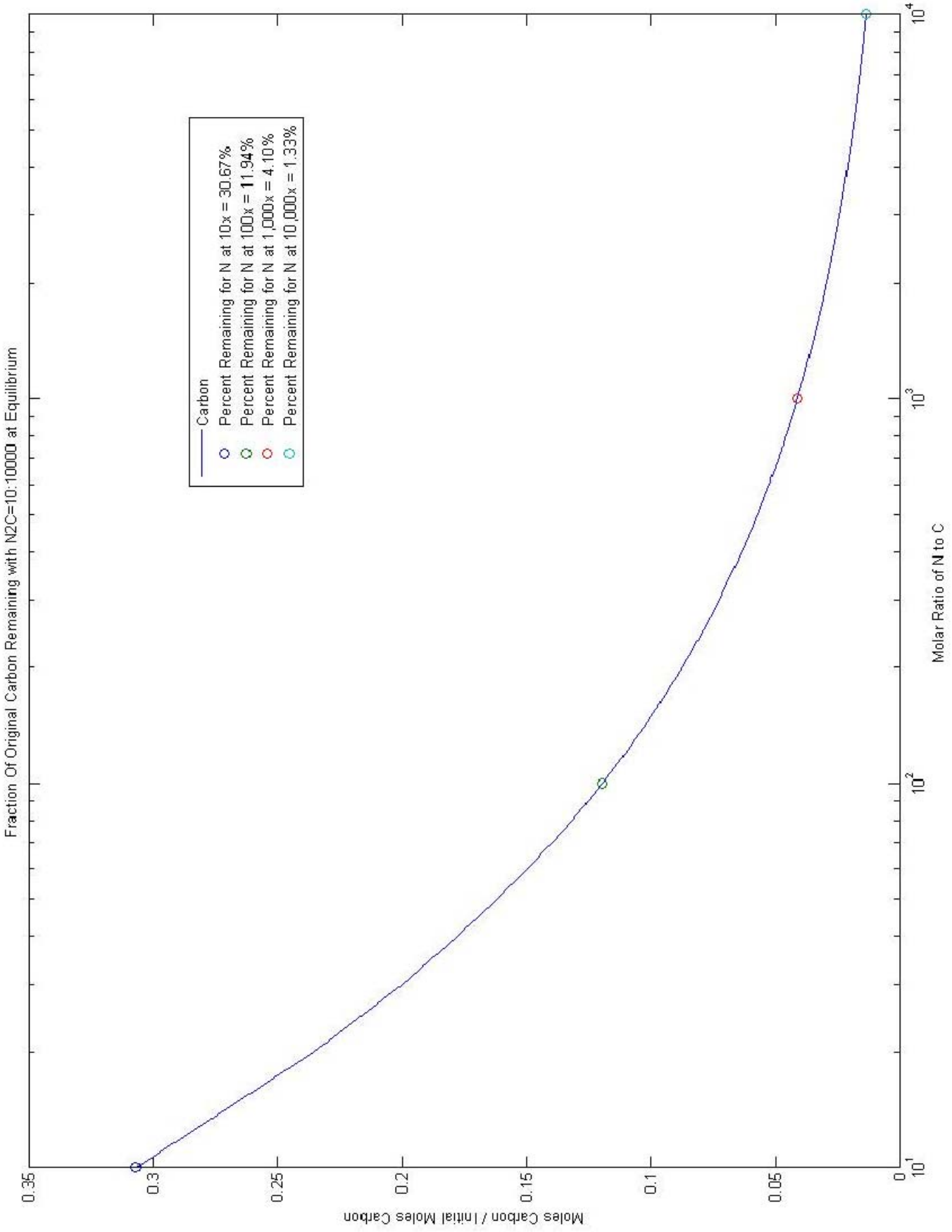
A.1.4 Case 2 Oxygen:Carbon 7:1



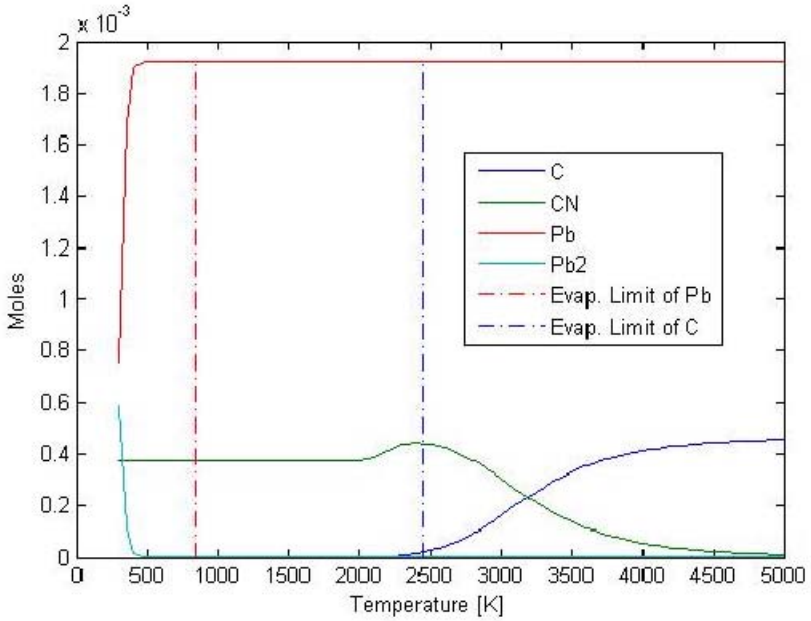
A.1.5 Case 3 Nitrogen:Carbon 1:1

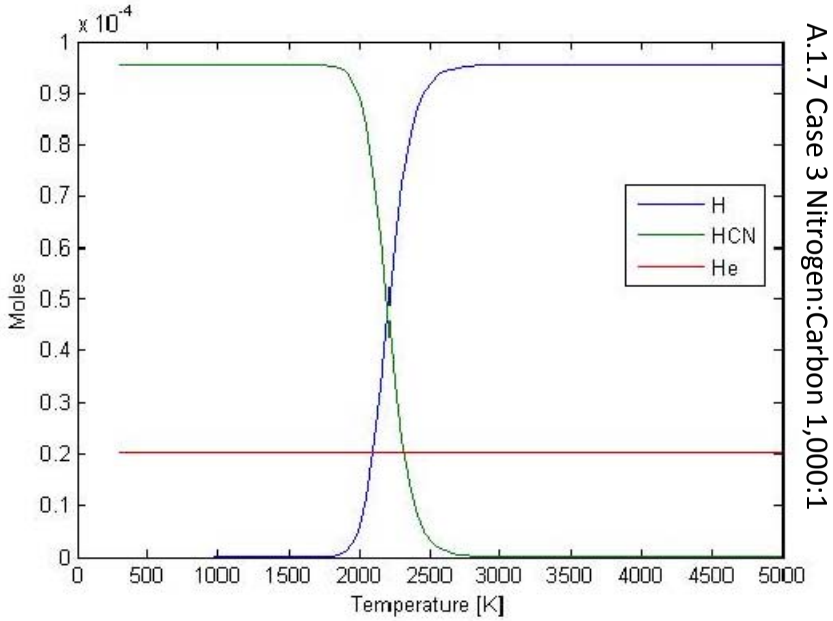


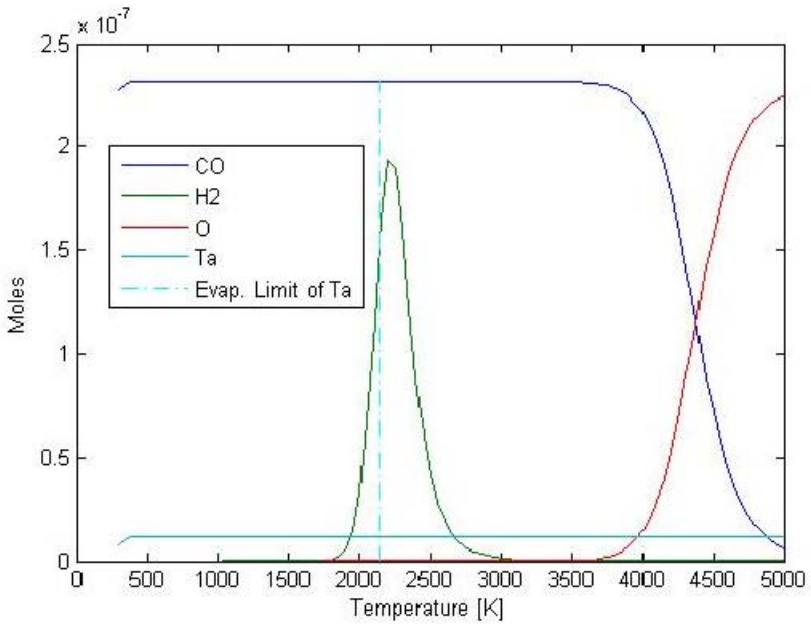
A.1.6 Case 3 Fraction of Origional Carbon Remaining Nitrogen:Carbon 10:1 to 10,000:1

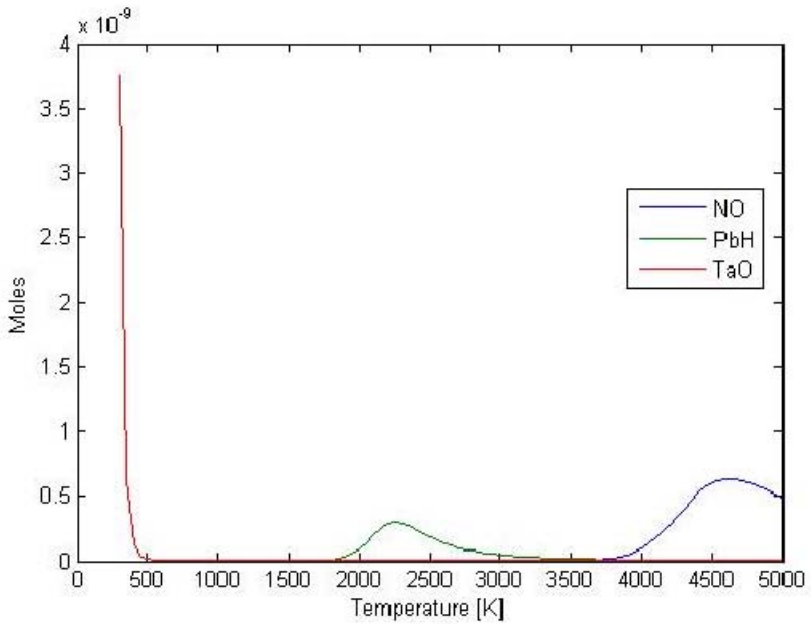


Major Species 1 Hohlraum + Xe and O2C=0 H2C=0 N2C=1000 at Equilibrium



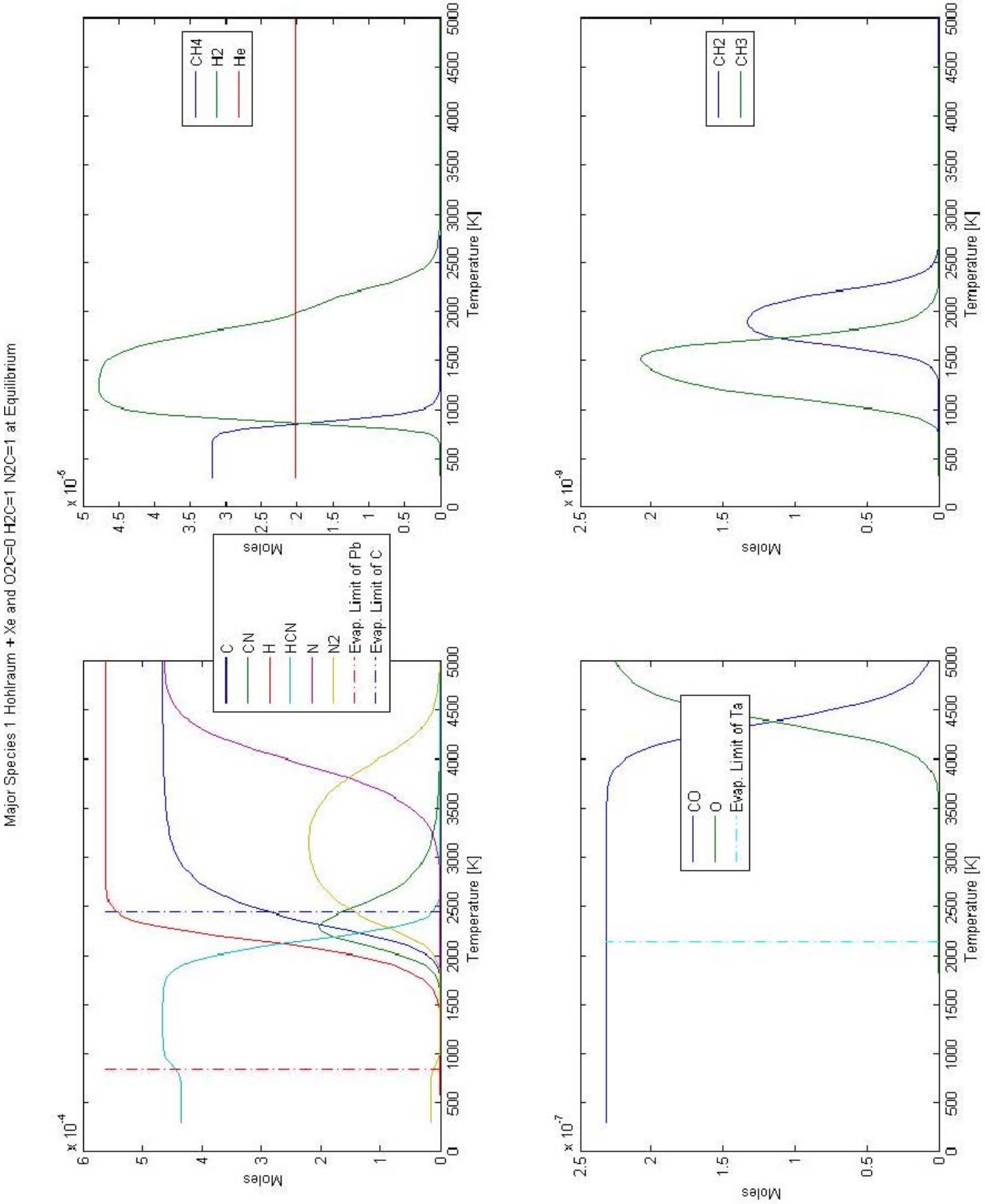




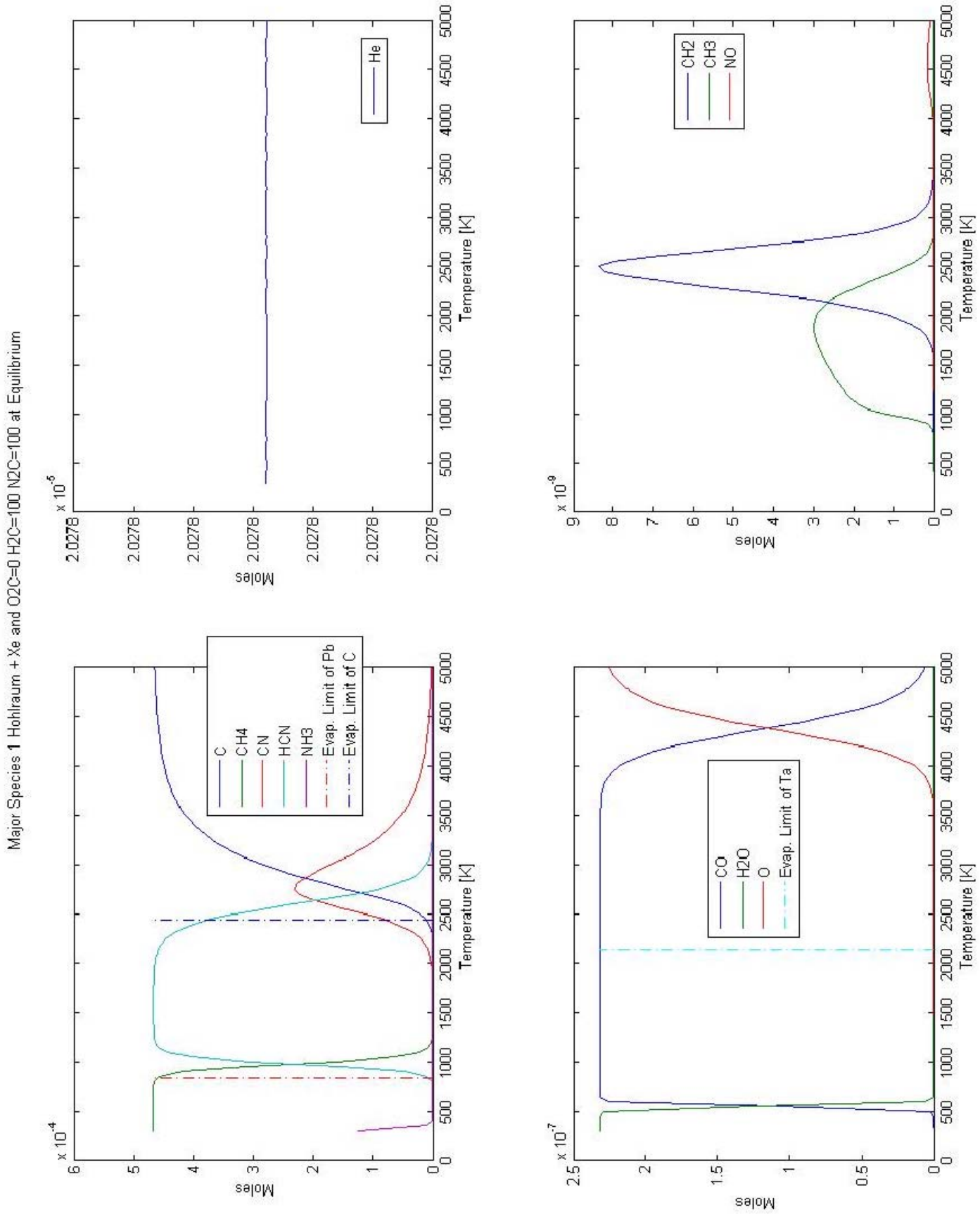


A.1.7 Case 3 Nitrogen:Carbon 1,000:1

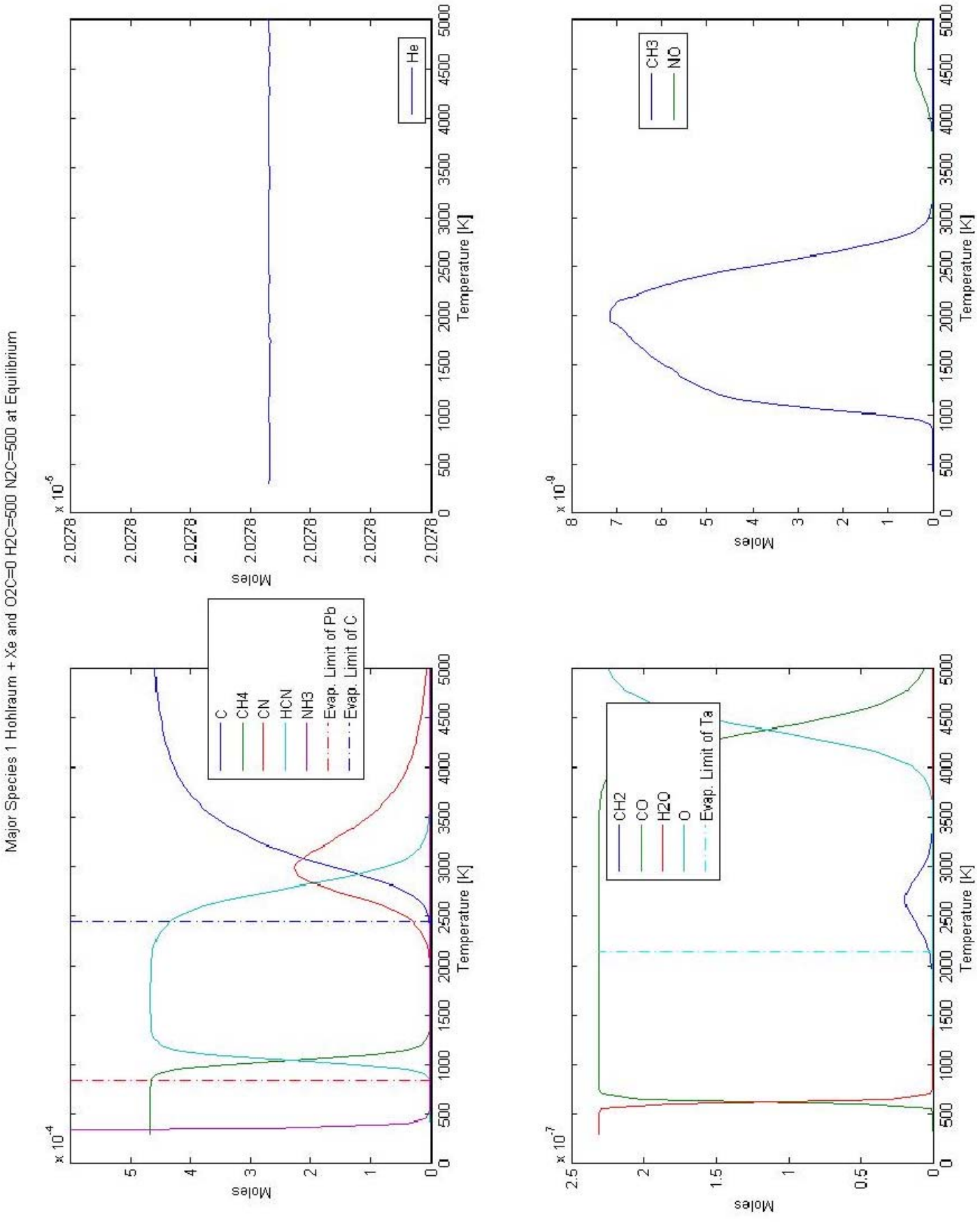
A.1.8 Case 4 Nitrogen:Carbon 1:1 Hydrogen:Carbon 1:1



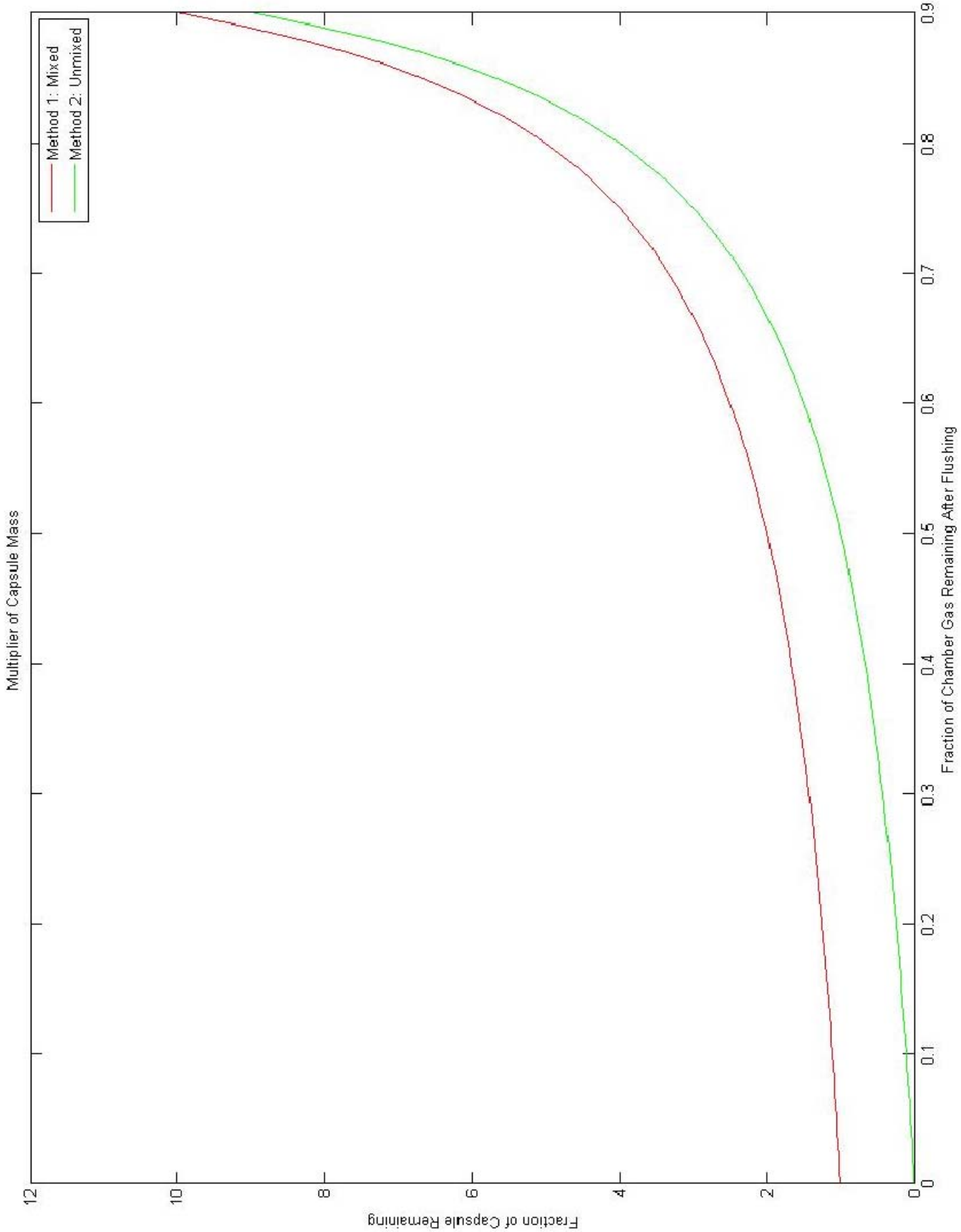
A.1.9 Case 4 Nitrogen:Carbon 100:1 Hydrogen:Carbon 100:1



A.1.10 Case 4 Nitrogen:Carbon 500:1 Hydrogen:Carbon 500:1



A.1.11 Fraction of Capsule Remaining



A.2 MatLab Code

A.2.1 Chamber Clearing Gas Equilibrium H, O, N, N-H Trials

```
close all
clear all
clc

%Define Gas Object
gas=IdealGasMix('lifechamber.xml');
gasID=newIdealGasMix('lifechamber.xml');

%Molar Masses of Elements Used
for Molar_Masses = 1:1
    MM  = molarMasses(gas);
    Nsp = nSpecies(gas);
    name = speciesNames(gas);

    H   = speciesIndex(gas,'H');
    He  = speciesIndex(gas,'He');
    C   = speciesIndex(gas,'C');
    N   = speciesIndex(gas,'N');
    O   = speciesIndex(gas,'O');
    Si  = speciesIndex(gas,'Si');
    Kr  = speciesIndex(gas,'Kr');
    Xe  = speciesIndex(gas,'Xe');
    Ta  = speciesIndex(gas,'Ta');
    Pb  = speciesIndex(gas,'Pb');

    CH2  = speciesIndex(gas,'CH2');          %Methylene
    CH3  = speciesIndex(gas,'CH3');          %Methyl group/radical
    CH4  = speciesIndex(gas,'CH4');
    CN  = speciesIndex(gas,'CN');            %Mace/Tear gas (Cyanide)
    CO  = speciesIndex(gas,'CO');
    CO2  = speciesIndex(gas,'CO2');
    C3H8  = speciesIndex(gas,'C3H8');        %Propane
    H2  = speciesIndex(gas,'H2');
    HCN  = speciesIndex(gas,'HCN');          %Hydrogen Cyanide
    H2O  = speciesIndex(gas,'H2O');
    NH3  = speciesIndex(gas,'NH3');          %Ammonia
    NO  = speciesIndex(gas,'NO');            %Nitric Oxide
    N2  = speciesIndex(gas,'N2');
    OH  = speciesIndex(gas,'OH');            %Hydroxide
    O2  = speciesIndex(gas,'O2');
    PbH  = speciesIndex(gas,'PbH');
    PbO  = speciesIndex(gas,'PbO');
    Pb2  = speciesIndex(gas,'Pb2');
    SiC4H12  = speciesIndex(gas,'SiC4H12');
    SiH  = speciesIndex(gas,'SiH');
    SiH2  = speciesIndex(gas,'SiH2');
    SiN  = speciesIndex(gas,'SiN');
    SiO  = speciesIndex(gas,'SiO');
    SiO2  = speciesIndex(gas,'SiO2');
    Si2  = speciesIndex(gas,'Si2');
    Si2N  = speciesIndex(gas,'Si2N');
    Si3  = speciesIndex(gas,'Si3');
    TaO  = speciesIndex(gas,'TaO');
```

```
    TaO2  = speciesIndex(gas,'TaO2');

    D  = Nsp+1;
    T  = Nsp+2;
    MM(D)  = 2.01410177785;
    MM(T)  = 3.01604927767;
end

m       = zeros(numel(MM),1);           %mass of Constituent Atoms
M       = zeros(numel(MM),1);           %Moles of Constituent Atoms
Temp    = 300;              %K
Ag      = 6.02214E+23;      %atoms/mole Avogadro's Number
e       = 1.60217646e-19;   %J/eV       Electron Charge
k       = 1.3806503e-23;    %J/K        Boltzman Constant
Vchamber= 65.5;             %m^3        Volume of Chamber
rhoXe   = 4;                %g/m^3      Initial Density Xe
vXe     = 1/rhoXe/1e-3;     %m^3/kg     Specific Volume Xe
m(Xe)   = rhoXe*Vchamber;   %g          Mass of Xe

%Hohlraum Components
for Hohlraum_Components = 1:1
    % All in mg
    Hm(H)  = 7.6e-4;
    Hm(D)  = .34/(MM(T)+MM(D))*MM(D);
    Hm(T)  = .34/(MM(T)+MM(D))*MM(T);
    Hm(He) = 0;
    Hm(C)  = 5.6;
    Hm(N)  = 9.7e-4;
    Hm(O)  = 3.7e-3;
    Hm(Si) = 0;
    Hm(Kr) = 0;
    Hm(Xe) = 0;
    Hm(Ta) = 2.1e-3;
    Hm(Pb) = 398;
    %Converting to g
    Hm     = Hm'*1e-3;          %g
end

%Adding Hohlraum Components to Chamber Mixture
m = m + Hm;                     %grams of Hohlraum elemets + Xe
HM = Hm./MM;                    %Moles of Hohlraum elements

%Adding Elements Initial Chamber Mixture to Tie up Carbon
%Initial Chamber Components
O2C     = 1;                %Oxygen to Carbon Ratio
H2C     = 0;                %Hydrogen to Carbon Ratio
N2C     = 1;                %Nitrogen to Carbon Ratio
M(Xe)   = m(Xe)/MM(Xe);     %moles      Moles of Xe
M(H)    = HM(C)*H2C;        %moles      Moles of H to add proportional to
moles of C
M(O)    = HM(C)*O2C;        %moles      Moles of O to add proportional to
moles of C
M(N)    = HM(C)*N2C;        %moles      Moles of N to add proportional to
moles of C

%Recalculating Specific Volume
```

```
m       = M.*MM;                 %g
v       = Vchamber/sum(m)/1e-3; %m^3/kg Updated Initial Specific Volume of
Chamber

%Fusion Reaction D+T -> He (assume 30% efficiency)
eff  = 0.3;
HM(He)= HM(He)+HM(D)*eff;
HM(D) = HM(D)*(1-eff);
HM(T) = HM(T)*(1-eff);

for shot = 1:1
    display(shot)
    M = M + HM;

    TotalMass = sum(M.*MM);

    constituents = strcat(  '  H:',num2str(M(H)+M(D)+M(T)),...
        ' He:',num2str(M(He)),...
        '  C:',num2str(M(C)),...
        '  N:',num2str(M(N)),...
        '  O:',num2str(M(O)),...
        ' Si:',num2str(M(Si)),...
        ' Kr:',num2str(M(Kr)),...
        ' Xe:',num2str(M(Xe)),...
        ' Ta:',num2str(M(Ta)),...
        ' Pb:',num2str(M(Pb)));
    M(H) = M(H)+M(D)+M(T);
    M(D) = 0;
    M(T) = 0;
    % Calculate Mole Fractions at Eq
    I = 0;
    Times_Stopped = 0;
    notreal = 0;
    MolesStart(:,1) = M(1:numel(M)-2);
    for Temp=300:50:5000
%         if Temp < 2500
%             II = 1;
%             Mt(:,II) = M(1:numel(M)-2);
%             Mt(HCN) = M(C);
%             Mt(H) = M(H)-M(C);
%             Mt(N) = M(N)-M(C);
%             Mt(C) = 0;
%         else
%             II = 2;
%             Mt(:,II) = M(1:numel(M)-2);
%         end
        I = I+1;
        stopped = 0;
        unstoppable = 0;
        while unstoppable == 0
            stopped = 0;
            state1  =
IdealGasMixState(gasID,'moleTP',MolesStart(:,1),Temp,101325);
            S1      = setState(state1,'V',v,'T',Temp);
            try
                state1eq = equilibrate(S1,'TV');
```

```
            catch
                Times_Stopped = Times_Stopped+1;
                stopped = 1;
            end
            if stopped == 1
                unstoppable = 0;
                MF(:,I) = 0;
            else
                MF(:,I) = getMoleFractions(state1eq);
                if sum(isnan(MF(:,I))) == 0
                    unstoppable = 1;
                elseif sum(isnan(MF(:,I)))>0
                    unstoppable = 0;
                    notreal = notreal+1;
                end
            end

        end
        TEQmass = sum(MF(:,I).*MM(1:numel(M)-2));
        Ratio = (TotalMass/TEQmass);
        EQMass(:,I,shot)  = MF(:,I).*MM(1:numel(M)-2).*Ratio;
        EQMoles(:,I,shot) = MF(:,I)*Ratio;
        MolesStart(:,I+1) = EQMoles(:,I);
        TT(I) = Temp;
        Temp
    end

    EQMass(:,:,shot) = EQMass(:,:,shot)*1000;       %convert from g to mg
    clc
    display(Times_Stopped)
    display(notreal)
    shots(shot) = shot;
    % M = M + sum(M);
    % M = M - HM*FXeA;
end

display(strcat('CO2 Produced Per year =
',num2str(HM(C)*MM(CO2)*10*60*60*24*365/1e3),' kg'))

%% Plotting Moles
for molefraction = 1:1
    close all
    for index = C:Xe
        maxEQMoles(index,1) = max(EQMoles(index,:,1));
    end
    maxmax = max(maxEQMoles(:,1));
    I1 = 0;
    I2 = 0;
    I3 = 0;
    I4 = 0;
    I5 = 0;
    I6 = 0;
    for index = C:Xe
        if (maxEQMoles(index) < 1e-2) && (maxEQMoles(index) >= 1e-4)
            I1=I1+1;
            graph1(I1,:) = EQMoles(index,:);
```

```
            legend1(I1)  = name(index);
        elseif (maxEQMoles(index) < 1e-4) && (maxEQMoles(index) >= 1e-6)
            I2=I2+1;
            graph2(I2,:) = EQMoles(index,:);
            legend2(I2)  = name(index);
        elseif (maxEQMoles(index) < 1e-6) && (maxEQMoles(index) >= 1e-8)
            I3=I3+1;
            graph3(I3,:) = EQMoles(index,:);
            legend3(I3)  = name(index);
        elseif (maxEQMoles(index) < 1e-8) && (maxEQMoles(index) >= 1e-10)
            I4=I4+1;
            graph4(I4,:) = EQMoles(index,:);
            legend4(I4)  = name(index);
        elseif (maxEQMoles(index) < 1e-10) && (maxEQMoles(index) > 0)
            I5=I5+1;
            graph5(I5,:) = EQMoles(index,:);
            legend5(I5)  = name(index);
        elseif (maxEQMoles(index) >= 1e-2)
            I6=I6+1;
            graph6(I6,:) = EQMoles(index,:);
            legend6(I6)  = name(index);
        end
    end

    if I1 == 0
        graph1 = 0;
        legend1 = 'No Data in this Range';
    end
    if I2 == 0
        graph2 = 0;
        legend2 = 'No Data in this Range';
    end
    if I3 == 0
        graph3 = 0;
        legend3 = 'No Data in this Range';
    end
    if I4 == 0
        graph4 = 0;
        legend4 = 'No Data in this Range';
    end

    figure
    subplot(2,2,1)
    if (numel(graph1(:,1)) <= 7)
        plot(TT,graph1(1:numel(graph1(:,1)),:))
    elseif (numel(graph1(:,1)) > 7) && (numel(graph1(:,1)) <= 14)
        plot(TT,graph1(1:7,:),TT,graph1(8:numel(legend1),:),'--')
    elseif (numel(graph1(:,1)) > 14) && (numel(graph1(:,1)) <= 21)
        plot(TT,graph1(1:7,:),TT,graph1(8:14,:),'--
',TT,graph1(15:numel(legend1),:),':')
    end
    hold on
    plot([838.6 838.6],[0 max(max(graph1))],'-.r')
    plot([2438.2 2438.2],[0 max(max(graph1))],'-.b')
    legend([legend1,'Evap. Limit of Pb','Evap. Limit of
C'],'location','best')
```

```
    xlabel('Temperature [K]')
    ylabel('Moles')

    subplot(2,2,2)
    if (numel(graph2(:,1)) <= 7)
        plot(TT,graph2(1:numel(graph2(:,1)),:))
    elseif (numel(graph2(:,1)) > 7) && (numel(graph2(:,1)) <= 14)
        plot(TT,graph2(1:7,:),TT,graph2(8:numel(legend2),:),'--')
    elseif (numel(graph2(:,1)) > 14) && (numel(graph2(:,1)) <= 21)
        plot(TT,graph2(1:7,:),TT,graph2(8:14,:),'--
',TT,graph2(15:numel(legend2),:),':')
    end
    legend(legend2,'location','best')
    xlabel('Temperature [K]')
    ylabel('Moles')
    %     title('Major Hydrogen and Carbon Consitiuents of Hohlraum at
Various Equilibrium Temperatures')

    subplot(2,2,3)
    if (numel(graph3(:,1)) <= 7)
        plot(TT,graph3(1:numel(graph3(:,1)),:))
    elseif (numel(graph3(:,1)) > 7) && (numel(graph3(:,1)) <= 14)
        plot(TT,graph3(1:7,:),TT,graph3(8:numel(legend3),:),'--')
    elseif (numel(graph3(:,1)) > 14) && (numel(graph3(:,1)) <= 21)
        plot(TT,graph3(1:7,:),TT,graph3(8:14,:),'--
',TT,graph3(15:numel(legend3),:),':')
    end
    hold on
    plot([2138.5 2138.5],[0 max(max(graph3))],'-.c')
    legend([legend3,'Evap. Limit of Ta'],'location','best')
    xlabel('Temperature [K]')
    ylabel('Moles')

    subplot(2,2,4)
    plot(TT,graph4)
    legend(legend4,'location','best')
    xlabel('Temperature [K]')
    ylabel('Moles')
    supertitle = strcat('Major Species 1 Hohlraum + Xe and
O2C=',num2str(O2C),' H2C=',num2str(H2C),' N2C=',num2str(N2C),' at
Equilibrium');
    suplabel( supertitle ,'t');

    figure
    subplot(1,2,1)
    plot(TT,graph6)
    legend(legend6,'location','best')
    xlabel('Temperature [K]')
    ylabel('Moles')
    axis([300 5000 0 max(max(graph6))*1.1])

    subplot(1,2,2)
    if (numel(graph5(:,1)) <= 7)
        semilogy(TT,graph5(1:numel(graph5(:,1)),:))
    elseif (numel(graph5(:,1)) > 7) && (numel(graph5(:,1)) <= 14)
        semilogy(TT,graph5(1:7,:),TT,graph5(8:numel(legend5),:),'--')
```

```
    elseif (numel(graph5(:,1)) > 14) && (numel(graph5(:,1)) <= 21)
        semilogy(TT,graph5(1:7,:),TT,graph5(8:14,:),'--
',TT,graph5(15:numel(legend5),:),':')
    end
    legend(legend5,'location','best')
    xlabel('Temperature [K]')
    ylabel('Moles')
    axis([300 5000 min(max(graph5,[],2))/1e2 max(max(graph5,[],2))])
end
%% Molecules formed, but in VERY low quantities, so Ignored
%C+ C- CHCO,ketyl C2H2,acetylene C2H2,vinylidene CH2CO,ketene C2H3,vinyl
CH3CN CH3CO,acetyl C2H4 C2H4O,ethylen
%CH3CHO,ethanal CH3COOH (HCOOH)2 C2H5 C2H6 CH3N2CH3 CH3OCH3 C2H5OH CCN CNC
%C2N2 C2O HCO HCO+ HCCN HNC HNO2 HNO3 HO2 HCHO,formaldehy HCOOH H2O2 H2O+
%H3O+ He+ N+ N- NH NH+ NH2 NH2OH NH4+ NO+ NO2 NO3 NCN N2H2 NH2NO2 N2H4 N2O3
%N2O4 N2O5 N3 N3H O+ O- OH+ OH- SiC SiC2 SiH3 SiH4 Si2 Si2C Si2N Si3

%O3 CH2OH CH3O CH3OH COOH NCO N2O
```

A.2.2 Evaporation Rate Calculation

```
clear all
close all
clc

Ag      = 6.02214E+23;      %atoms/mole Avogadro's Number
k       = 1.3806503e-23;    %J/K        Boltzman Constant
R       = 2.5;              %m          Radius of Chamber
SA      = 4*pi*R^2;         %m^2        Surfact Area of Chamber

C  = 1;
Pb = 2;
Ta = 3;
Hg = 4;

% Mass in Hohlraum
m(C)  = 5.6e-3;     %g
m(Pb) = 0.398;      %g
m(Ta) = 2.1e-6;     %g

ShotRate = 10;      %Shots per second
m = m*ShotRate;

%Constants For Rate of Evaporation of Metals
%C(s) : A = 14.06, B =38570, C = .3056
%Pb(l): A = 10.69, B =9600,  C = .9242
%Ta(s): A = 13.00, B =40210, C = .8947
a(C)  = 14.06;
b(C)  = 38570;
c(C)  = .3056;

a(Pb) = 10.69;
b(Pb) = 9600;
c(Pb) = .9242;

a(Ta) = 13.00;
b(Ta) = 40210;
c(Ta) = .8947;

Tmax = 5000;
Tmin = 300;
I = Ta;
Terror = 1;
% SA = 20;
while abs(Terror)>1e-9
    Tg = (Tmax+Tmin)/2;
    %Using data fits from The American Institute of Physics Handbook 3rd ED
    W(I)   = 10^(a(I)-b(I)/Tg-0.5*log10(Tg)+c(I)); %Mass Flux Rate inside
Chamber g/m^2-s
    ER(I)  = W(I)*SA;                              %Evaporation Rate inside
the Chamber

    if ER(I) < m(I)
        Tmax = Tmax;
        Tmin = Tg;
```

```
    else
        Tmax = Tg;
        Tmin = Tmin;
    end
    Terror    = (ER(I)-m(I))/m(I);
end
Tg
TC = Tg-273
```